1,2-Cyclohexanedicarboxylic acid, octyl 3-phenylpropyl ester

Inchi: InChI=1S/C25H38O4/c1-2-3-4-5-6-12-19-28-24(26)22-17-10-11-18-23(22)25(27)29-20-1

InchiKey: HDJDOQGIINBKND-UHFFFAOYSA-N

Formula: C25H38O4

SMILES: CCCCCCCCOC(=O)C1CCCCC1C(=O)OCCCc1ccccc1

Mol. weight [g/mol]: 402.57

Physical Properties

Property code	Value	Unit	Source
gf	-179.07	kJ/mol	Joback Method
hf	-778.42	kJ/mol	Joback Method
hfus	53.03	kJ/mol	Joback Method
hvap	91.95	kJ/mol	Joback Method
log10ws	-6.53		Crippen Method
logp	5.872		Crippen Method
mcvol	343.370	ml/mol	McGowan Method
pc	1094.27	kPa	Joback Method
rinpol	2948.00		NIST Webbook
tb	965.54	K	Joback Method
tc	1185.74	K	Joback Method
tf	545.39	K	Joback Method
vc	1.308	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1181.34	J/mol×K	965.54	Joback Method
cpg	1249.69	J/mol×K	1149.04	Joback Method
cpg	1239.25	J/mol×K	1112.34	Joback Method
cpg	1227.25	J/mol×K	1075.64	Joback Method
cpg	1213.62	J/mol×K	1038.94	Joback Method
cpg	1198.34	J/mol×K	1002.24	Joback Method
cpg	1258.62	J/mol×K	1185.74	Joback Method
dvisc	0.0000356	Pa×s	965.54	Joback Method
dvisc	0.0000465	Pa×s	895.51	Joback Method

dvisc	0.0000636	Pa×s	825.49	Joback Method
dvisc	0.0000923	Pa×s	755.46	Joback Method
dvisc	0.0001444	Pa×s	685.44	Joback Method
dvisc	0.0002503	Pa×s	615.41	Joback Method
dvisc	0.0004993	Pa×s	545.39	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339499&Units=SI

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume